ISBN: 978-3-95450-168-7 doi:10.18429/JACoW-IPAC2015-MOPMA045

CONCEPTUAL DIFFICULTIES OF A THERMODYNAMICS DESCRIPTION OF CHARGED-PARTICLE BEAMS *

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Abstract

We review the existing phenomenological theories of emittance growth with and without entropy terms and re-examine the condition for thermal equipartitioning in an unbunched charged-particle beam. The model incorporates linear space charge and a uniform-focusing lattice. Because of non-extensitivity of the transverse ("thermal") energy and the absence of a classical heat bath, we conclude that a rigorous classical thermodynamics treatment of charged-particle beams is not possible. In particular, the postulated relationships between the rms emittance and temperature and entropy must be qualified.

INTRODUCTION

Lapostolle suggested some 45 years ago [1] that a thermodynamic model may apply to the observed emittance exchanges between degrees of freedom in intense charged-particle beams (e.g., proton linacs at CERN). He went further to comment that heat flow may occur between degrees of freedom corresponding to different temperatures; under these circumstances, entropy would increase and emittance blow up in an irreversible manner.

Since Lapostolle's work, phenomenological theories of emittance growth have been developed by Wangler, Reiser, and others [2, 3]. Furthermore, a connection between rms emittance and entropy had been suggested by Lawson, Lapostolle and Gluckstern in 1973 [4]. Although the original work by Wangler et al does not address reversibility, an extension of the theory by O'Shea [5] predicts a connection between entropy changes and reversible and irreversible rms emittance growth. However, a thermodynamic framework for describing beam dynamics has neither been theoretically examined in detail nor tested in simulations.

Recent work by Hofmann and Boine-Frankenheim [6] emphasizes computational aspects of emittance and entropy growth. Their simulation studies focus on the role of grid resolution and numerical collisions on (6D) rms emittance and entropy growth in 3D beams confined by a periodic potential. Moreover, Hofmann and Boine-Frankenheim compare the numerical results to the predictions of a stochastic model developed by Struckmeier [7] based on temperature anisotropy and the effect of using macro-particles.

ENTROPY AND EMITTANCE GROWTH

In the phenomenological theory of Wangler et al [2, 3], the rate of change of normalized rms emittance (squared) in an unbunched beam is described by the equation

$$\frac{d\tilde{\varepsilon}_n^2}{dz} = -\frac{1}{8}\beta^2\gamma^2 \left\langle x^2 \right\rangle K \frac{d}{dz}\left[\frac{U(z)}{W_0}\right], \qquad (1)$$

where z is the axial coordinate, $U(z) = W - W_u$ the difference between field energies per unit length of the actual beam distribution and the equivalent uniform distribution, i.e., the Kapchinskij-Vladimirskij (K-V) beam [3], and W_0 is the space-charge field energy per unit length inside the boundary of the equivalent K-V beam. The excess energy $U(z)$, or *free energy*, is available for the beam to thermalize. The symbol K represents the generalized beam perveance, which is proportional to current; $\left\langle x^2 \right\rangle = \left\langle y^2 \right\rangle$ is the squared rms transverse dimension at z, and the rest of the quantities have the standard meanings from special relativity.

No statement about *reversibility* is made in the original derivation of eq. (1). In O'Shea's work [5], though, eq. (1) is qualified as one *valid when the entropy change is zero* and, therefore, when the rms emittance change is in principle *reversible* by the application of *appropriate* forces. The reversibility, however, will depend on our ability to apply corrective forces with the same fine resolution that lead us to conclude that no entropy growth occurred. In many practical situations, this resolution is not possible and, hence, we must conclude that entropy in fact increased and emittance change is irreversible.

The normalized information entropy, S_n, in O'Shea's work is related to the normalized transverse rms emittance. For a 2-D beam we have [4]:

$$S_n(z) \equiv \frac{S_2(z)}{k_B N L} = \ln[\tilde{\varepsilon}_n(z)] + \ln[C(z)] - \ln[A_2], \qquad (2)$$

where k_B is Boltzmann's constant, N is the number of beam particles per unit length, L, the bunch's length, is $L >>$ transverse dimension. $C(z)$ depends on the form of the phase-space particle distribution at z, and A_2 corresponds to the size of the grid cell for the computation, or the experimental resolution of the measuring device. Equation (2) tells us that it is possible to have rms emittance growth while entropy remains constant because the evolution of $C(z)$ may compensate for the growth. By the same token, it is possible for rms emittance to decrease while entropy increases. The value of $C(z)$ at $z = 0$, the start of the simulation or experiment, is denoted by C_0. For the widely used K-V distribution, for example, $C_0 = \pi$; for a thermal (Gaussian) distribution, $C_0 = \sqrt{2}\pi^{3/2}$ [4], more than twice the value for the K-V distribution.

* Work supported by U.S. Department of Energy

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The inclusion of the entropy term S_n in eq. (1) by O'Shea [5] leads to

$$\frac{d\tilde{\varepsilon}_n^2}{dz} = -\frac{2\gamma\left\langle x^2\right\rangle}{mc^2NL}\left[\frac{d\hat{U}}{dz} - T_{eff}\frac{dS_n}{dz}\right], \qquad (3)$$

where the term $\hat{U}$ comprises contributions from self-field and transverse kinetic energy changes relative to the effective linear models (K-V beam distribution for the transverse plane) as in eq. (1). T_{eff} is an effective transverse temperature for the beam given by:

$$T_{eff} = \frac{mc^2\tilde{\varepsilon}_n^2}{k_B\gamma\left\langle x^2\right\rangle}. \qquad (4)$$

A "generalized" free-energy function is defined by O'Shea as $\hat{F} = \hat{U} - T_{eff}S_n$, which is reminiscent of the Helmholtz free-energy of classical thermodynamics. Apparently, however, T_{eff} in eq. (3) is factored out as a constant when taking the derivative $d\hat{F}/dz$. The entropy term S_n in the original formulation [5], on the other hand, is the entropy of the average slice in the bunch; for an unbunched beam, it is implied that NLS_n is the entropy of the entire beam.

Returning to eq. (3), in the limit $T_{eff} = 0$ (cold beam), the Maxwell-Boltzmann distribution is a uniform distribution, and eq. (3) reduces to eq. (1). In the opposite limit of emittance-dominated beam, $T_{eff}S_n >> \hat{U}$. The original phenomenological model of Wangler et al [2, 3] is applicable to *space-charge dominated* beam transport where rms emittance growth is driven by space charge forces and the beam evolves to one whose distribution is close to a K-V distribution. Naturally, this rms emittance growth is largest for beam transport with small values of the tune depression, i.e., strongly space-charge dominated beams [3]. The more general model embedded in eq. (3) is in principle applicable to beam transport with *any* value of tune depression.

EQUIPARTITIONING AND EXTENSITIVITY

Temperature anisotropy leads to flow of thermal energy from the "hot" to the "cold" degrees of freedon. In general, the equipartitioning condition can be expressed as [3, 8, 9]:

$$\tilde{\varepsilon}_x k_x = \tilde{\varepsilon}_y k_y = \tilde{\varepsilon}_z k_z, \qquad (5)$$

where $\tilde{\varepsilon}_{x,y,z}$ represent rms emittances, and $k_{x,y,z}$ are wavenumbers associated with particle oscillations in a beam transport model with uniform external focusing *and* (linear) space charge. For simplicity, we assume that $\tilde{\varepsilon}_x = \tilde{\varepsilon}_y$, as in Appendix 4 of [3].

The transverse rms emittance, $\tilde{\varepsilon}_x$, has been related to temperature [3] and also to entropy [4, 5, 7]. The first case is justified by the use of $\tilde{\varepsilon}_x$ as a measure of the beam divergence which results from transverse kinetic ("thermal") energy, while the connection to entropy would arise from the identification of $\tilde{\varepsilon}_x$ with phase-space area and the number of dynamical "states" associated with that area.

But in classical equilibrium thermodynamics temperature is an *intensive* variable while entropy is an *extensive* variable. Extensive variables scale linearly with the number of particles in the system, while intensive variables remain constant. In most contexts, it is clear what parameters should be classified as intensive and which as extensive. Thus, a classical gas occupying a volume V (extensive variable) and at equilibrium temperature T and pressure p (T, p intensive variables) can be partitioned into two equal volumes with a wall without changing T,p.

It is straightforward to show that a charged-particle beam is a non-extensive system, i.e., that the energy *per particle* will depend on the number of particles. As before, we consider an unbunched beam in a uniform-focusing channel. The total average energy *per particle* can be written as the sum of contributions from the kinetic energy of transverse motion, the potential energy associated with external focusing, and the internal potential energy from linear space charge. This average is over one wavelength of betatron oscillations including space charge, as presented in Sec. 6.2.1 in [3]. Explicitly,

$$e_T = e_k + e_p + e_s = e_T = e_{k0}\left[2 - \frac{\chi}{2}\left(1 - 4\ln\frac{b}{a}\right)\right], \qquad (6)$$

where (see chapter 6 in Ref. [3]),

$$e_k = e_{k0}(1-\chi), \quad e_{k0} \equiv \gamma m(vak_0/2)^2, \qquad (7)$$

$$e_p = e_{k0}, \quad e_s = \frac{e_{k0}}{2}\chi\left[1 + 4\ln(b/a)\right]. \qquad (8)$$

In eqs (6-8), $a = 2\sqrt{\langle x^2\rangle}$ is the effective matched beam radius, b is the vacuum pipe radius, k_0 is the (constant) wavenumber of zero-current betatron oscillations (i.e., it represents external focusing), γ is the relativistic mass factor, v is the beam axial speed, $v >> v_x$, and χ is the *space charge (SC) intensity parameter* defined by $\chi = K/(a^2k_0^2)$ [3]. Notice that e_{k0} depends on χ through the beam radius a. This radius must satisfy the matching condition, $a = 2\sqrt{\tilde{\varepsilon}_x/k}$, where $k \equiv k_x = k_y$ is the depressed wavenumber of betatron oscillations. In the limit of "zero" current, $a = a_0 = 2\sqrt{\tilde{\varepsilon}_x/k_0}$. Furthermore, the kinetic energy of transverse motion is assumed to be small compared to the net kinetic energy even for non-relativistic beams, i.e. $e_k << mv^2/2$.

Returning to the expressions for the energy per particle, eqs. (6-8), we find that in the limit of "zero" current ($\chi = 0$) we can write

$$e_T = 2e_{k0} = 2\gamma m(va_0k_0/2)^2 = 2\gamma mv^2\tilde{\varepsilon}_x k_0. \qquad (9)$$

With "zero" current, there would be no meaning to the concept of extensive system, but we can still imagine changing the number of particles and neglecting space charge altogether. With constant focusing, we could postulate that emittance is an *intensive* variable, i.e. a temperature-like variable; but more generally, $\tilde{\varepsilon}_x k_0$ should be the intensive parameter. Therefore, eq. (5) is, at best, an approximate condition for thermal *kinetic* equilibrium when space charge is

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negligible, i.e. when k_0 and not the depressed wavenumber k characterizes particle oscillations in the beam.

In the limit of space-charge dominated transport where $\chi = 1$, or $\epsilon = 0$, on the other hand, the total energy per particle is,

$$e_T = e_{k0}\left[\frac{3}{2} + 2\ln\frac{b}{a}\right]. \tag{10}$$

Since $\ln(b/a)$ is of order unity, we can write, in the limit of space-charge dominated transport, $e_T \sim \gamma m v^2 K$, which is just a statement of the non-extensitivity of the total transverse energy as K, the beam perveance, is proportional to the beam current. In conclusion, charged-particle beams are not normal thermodynamical systems because the total transverse energy per particle is not an intensive variable, and, furthermore emittance and other parameters such as χ are neither intensive nor extensive so cannot function as thermodynamical variables.

DISCUSSION

The theories of rms emittance growth discussed above are called "phenomenological" as they do not include explicitly a physical mechanism or time scale for the emittance evolution. Thus, the theories allow a calculation of the *net* change in rms emittance from an initial non-equilibrium distribution [3]. The theory embedded in eq. (1), for example, has been verified in computer simulations and in experiments at the University of Maryland and Los Alamos National Lab [10, 11]. However, no tests of the extended theory behind eq. (3) have been attempted. It is not obvious, in this regard, that computer simulations (which yield *reversible* dynamics over not-too-long runs and with enough resolution), can predict *irreversibility* of rms emittance growth, or whether entropy as defined in [4–7], or otherwise, can guide the simulations. More importantly, although classical thermodynamics is also a phenomenological theory, no rigorous connection of emittance evolution to standard thermodynamics seems possible despite the use of similar language. A simple scenario, the free expansion of a charged-particle beam, can illustrate the pitfalls of attempting a classical thermodynamics description and of associating emittance with temperature or entropy.

The rms emittance of an expanding K-V beam is unchanged, but the process is clearly irreversible. Thus, the entropy term in eq. (3) should exactly balance the energy term $\hat{U}$. Moreover, there is no *heat* exchange as in the standard free expansion of an ideal gas after the removal of a partition in a divided (and thermally isolated) container. Unlike the ideal gas, however, the effective temperature - eq. (4) - decreases as the beam expands. Alternatively, we can compare the free expansion of the beam with the *adiabatic* expansion of an ideal gas whereby, for example, the thermally-isolated gas works against a sliding piston and gets colder; but then the question arises about defining *work* and *heat* for processes in a charged-particle beam. In short, it is not clear that a beam can undergo the equivalent of isothermal and adiabatic expansions of ideal gases.

In a mathematical context, it is the non-extensitivity of the total energy and entropy in charged-particle beams (and gravitational systems as well) which in principle disallows a standard thermodynamics treatment. This extensitivity property is a fundamental requirement that leads to thermodynamics relations such as the Gibbs-Duhen equation and the very definition of temperature in normal thermodynamics systems, as discussed in many textbooks (see e.g. [12]). Nevertheless, a kinetic treatment of charged-particle beams as non-neutral plasmas is always possible, but it is in general not possible to equate kinetic and thermodynamic temperatures.

Regarding entropy, any attempt at a rigorous statistical-mechanics definition for the description of charged-particle beams is met with difficulties. Thus, it would seem that because the K-V distribution is a *micro-canonical* distribution, a micro-canonical entropy can be defined. If $\Omega(E)$ is proportional to the volume in phase space at a (constant) total energy E, the micro-canonical entropy is $S(E) = k_B \ln\Omega(E)$, where $\Omega(E)$ is also interpreted as a thermodynamic probability. The entropy is extensive, i.e, additive, only if the system can be subdivided into n subsystems such that $\Omega = \Omega_1\Omega_2...\Omega_n$, i.e. if the subsystems are *statistically independent*. (In the micro-canonical ensemble, the interaction among the system's parts is all that counts.) But a charged-particle beam cannot be arbitrarily partitioned into statistically independent sub-systems in the same way that an ideal gas can. The latter is a necessary condition to assert that all microscopic states, compatible with a constant total energy, are equally accessible, i.e., have the same probability.

Another widely used concept in describing charged-particle beams is the Boltzmann factor $\exp(-H/k_BT)$; here H can be considered as the transverse Hamiltonian and T as the transverse temperature (normally much larger than the longitudinal temperature [3].) The *canonical ensemble* is implicit in this picture, but no discernible *heat bath*, which is a key component of the ensemble, is ever present! Therefore T cannot be a thermodynamic temperature, but simply a kinetic parameter characterizing the spread of energies in a model distribution. More importantly, a beam may evolve towards an equilibrium characterized by an effective Maxwell-Boltzmann distribution, but such equilibrium cannot be rigorously described as thermodynamic equilibrium.

In our opinion, understanding the fundamental issue of reversibility/irreversibility of rms emittance growth in beams requires a detailed study of the mechanisms involved. Such a study would yield time scales and help guide both simulations and experiments. A phenomenological picture may still be useful, perhaps one based on constitutive relations similar to those introduced in fluid dynamics or electromagnetic theory. Nevertheless, we cannot discount the role of entropy and other concepts from statistical thermodynamics for a better description of charged-particle beam dynamics.

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